**Dr. George Geromichalos, Ph.D.** Head in Cell Culture Molecular Modeling & **Drug Design Dept. Symeonidion Research Center, Theagenion Cancer Hospital, Thessaloniki,** Greece

 Research on cytotoxic/cytostatic activity of new experimental and well-established chemotherapeutic drugs or their combination

 Cell cycle analysis, study of signal transduction pathways and their relation to cytotoxicity or apoptosis

Study of the genes that are related to the growth or suppression of cancer growth

Research & Development of new drugs with improved toxicity pattern, increased anticancer activity and better selectivity, through modifying the structure of known functional molecules

- Research on the bioactivity of many phytochemical compounds (bioactive and functional molecules) derived from a variety of medicinal plants
- Elucidation of the mechanism of action in molecular and cellular level

 Virtual high-throughput screening and study of the structure of the active or binding site of a plethora of new all-promising target-proteins in the research field of cancer therapy as well as of many other diseases

Study on the chemical structure and biologic activity of transition compounds as well as hybrid steroidal compounds

 Design of multi-target drugs to be effective in controlling complex diseases as cancer

### My interest is focused

in the development of new therapeutic strategies based on both theoretical and experimental methods in order to evaluate new compounds with possible anticancer or other activity, and the development of more effective drugs with less side-effects Rational drug discovery via "computer-assisted combinatorial method" is used for

 Understanding of molecular interactions between active anticancer drugs and their molecular and cellular targets in the signal transduction pathways they participate

Discovery new therapeutic strategies based in new knowledge about molecular modeling and combinatorial chemistry (computer aided drug design) Research & development of new anticancer drugs (and other drugs)with:

- Improved toxicity pattern
- Increased anticancer activity and better selectivity
- Modifying the structure of known functional molecules
- study of signal transduction pathways and their relation to cytotoxicity or apoptosis

#### In vitro cell cultures

- Bank of 40 established cell lines in liquid nitrogen (from human & mouse solid tumors and also lymphomas and leukemia)
- **Cell culture**

is a useful model for the study of signal transduction pathways, as targets for new anticancer drugs and the elucidation of their mechanism of action at both molecular and cellular level, as well as the comparison of these compounds with other fully established anticancer agents used in clinical practice.

### **Cell culture**

With the aid of in vitro models, it is investigated the cytotoxic/cytostatic activity, alone or in combination, of experimental and known anticancer agents, that may play a role in various sites of the signal transduction pathways and be targets for the new drugs

## **In Silico**

Modern in silico computational chemistry and molecular modeling techniques aiming:

- Discovery of targeted rational computer-aided drug design molecules
- Molecular modeling of newly synthesized compounds with possible anticancer or other activity

Study of the structure of the active or binding site of a plethora of new all-promising targetproteins in the research field of cancer therapy & therapy of other diseases

Investigation at a molecular level the correlation of novel agents with cellular entities of cancer cells or the protein targets of other diseased cells Definition of the possible correlation between chemical and electronic structure of the studied compounds and their anticancer or other activity with view to developing more active drugs with enhanced toxicity and anticancer profile and more selectivity

# **In Silico Techniques**

- Computational chemistry
- Quantum-chemical computations (QM-based Drug Discovery)
- Virtual high-throughput screening (vHTS)
- Molecular docking and dynamics techniques
- Application on bio- & chemo-informatics techniques
- Combinatorial chemistry ("CombiChem")

- Structure-based drug design (SBDD)
- Fragment-based drug design (FBDD)
- Ligand-based drug design
- In silico ADME/T prediction
- Homology modeling
- Pharmacophore modeling
- Quantitative structure-activity relationship (QSAR)

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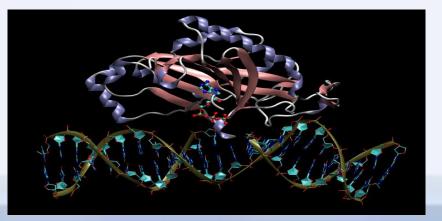


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